F 689 – Mecânica Quântica I

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Aula 25

Aulas passadas

Definição geral de momento angular: 3 operadores tais que

$$\boxed{\begin{aligned}[J_x, J_y] &= i\hbar J_z \\ [J_y, J_z] &= i\hbar J_x \\ [J_z, J_x] &= i\hbar J_y\end{aligned}}$$

Módulo quadrado do momento angular: $J^2 = J_x^2 + J_y^2 + J_z^2$

$$\left[J^2, J_i\right] = 0$$

Assim, escolheremos J^2 e, por exemplo, J_z , para formar um par de operadores que comutam.

Aulas passadas

Auto-vetores simultâneos de J^2, J_z :

$$J^2 \left|k, j, m\right\rangle = j\,(j+1)\,\hbar^2 \left|k, j, m\right\rangle$$
$$J_z \left|k, j, m\right\rangle = m\hbar \left|k, j, m\right\rangle$$

onde k distingue entre os auto-vetores diferentes com mesmo (j,m).
Os valores possíveis de (j,m) são:

$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \frac{5}{2}, \ldots$$
$$m = -j, -j+1, \ldots, j-1, j$$

Para cada j, há $2j+1$ valores possíveis de m.

Aula passada

Base padrão: $[k = 1, 2, \ldots, g(j)]$ $\langle k', j', m' | k, j, m \rangle = \delta_{k,k'} \delta_{j,j'} \delta_{m,m'}$

$$\sum_j \sum_{m=-j}^{+j} \sum_{k=1}^{g(j)} |k, j, m\rangle \langle k, j, m| = \mathbb{1}$$

Ação universal dos operadores **J** na base padrão:

$$J^2 |k, j, m\rangle = j(j+1)\hbar^2 |k, j, m\rangle$$
$$J_z |k, j, m\rangle = m\hbar |k, j, m\rangle$$
$$J_+ |k, j, m\rangle = \sqrt{j(j+1) - m(m+1)}\hbar |k, j, m+1\rangle$$
$$J_- |k, j, m\rangle = \sqrt{j(j+1) - m(m-1)}\hbar |k, j, m-1\rangle$$

Aula passada

Momento angular orbital: **L = R x P**

Operadores **L** na representação de posição (em coordenadas esféricas r, θ, ϕ):

$$L_x = i\hbar\left(\sin\theta\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right)$$

$$L_y = i\hbar\left(-\cos\theta\frac{\partial}{\partial\theta} + \frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right)$$

$$L_\pm = \hbar e^{\pm i\phi}\left(\pm\frac{\partial}{\partial\theta} + \frac{i}{\tan\theta}\frac{\partial}{\partial\phi}\right)$$

$$L_z = -i\hbar\frac{\partial}{\partial\phi}$$

$$L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

Aula passada

Auto-funções simultâneas de L^2 e L_z:

$$-\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(r,\theta,\phi)=l(l+1)\psi(r,\theta,\phi)$$

$$-i\frac{\partial}{\partial\phi}\psi(r,\theta,\phi)=m\psi(r,\theta,\phi)$$

m e l só podem assumir valores inteiros.

$$\psi(r,\theta,\phi)=R_{kl}(r)\,Y_{lm}(\theta,\phi)$$

$$Y_{\ell m}(\theta,\phi)=z_{\ell m}(\theta)\,\frac{e^{im\phi}}{\sqrt{2\pi}}$$

$$Y_{ll}(\theta,\phi)=\frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)!}{4\pi}}(\sin\theta)^l e^{il\phi}$$

$$Y_{lm}(\theta,\phi)=\left[\frac{L_-}{\hbar\sqrt{l(l+1)-m(m-1)}}\right]^{(l-m)}Y_{ll}(\theta,\phi)$$

Os $Y_{lm}(\theta,\phi)$ são chamados de harmônicos esféricos.

Aula passada

Ortonormalização: $$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta Y^*_{l'm'}\left(\theta,\phi\right) Y_{lm}\left(\theta,\phi\right) = \delta_{l,l'}\delta_{m,m'}$$

Expansão de funções de (θ,ϕ): $$f\left(\theta,\phi\right) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} c_{l,m} Y_{lm}\left(\theta,\phi\right)$$

$$c_{l,m} = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta d\theta Y^*_{lm}\left(\theta,\phi\right) f\left(\theta,\phi\right)$$

Fechamento: $$\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y^*_{lm}\left(\theta',\phi'\right) Y_{lm}\left(\theta,\phi\right) = \frac{1}{\sin\theta}\delta\left(\theta-\theta'\right)\delta\left(\phi-\phi'\right)$$

Complexo conjugado: $$Y^*_{l,m}\left(\theta,\phi\right) = \left(-1\right)^m Y_{l,-m}\left(\theta,\phi\right)$$

Inversão espacial: **r→-r** $$Y_{l,m}\left(\pi-\theta,\phi+\pi\right) = \left(-1\right)^l Y_{l,m}\left(\theta,\phi\right)$$

Expansão numa base padrão

Suponha dada uma função de estado: $\psi\left(r,\theta,\phi\right)$ $\rightarrow$ NORMALIZADA

EXPANDIR NUMA BASE PADRÃO: $|k,\ell,m\rangle$

$$|\psi\rangle = \sum_{k=1}^{g(\ell)} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \underbrace{\langle k\ell m|\psi\rangle}_{C_{k\ell m}} |k\ell m\rangle = \sum_k \sum_\ell \sum_m C_{k\ell m} |k,\ell,m\rangle$$

EM TERMOS DE FUNÇÃO DE ONDA:

$$\langle r,\theta,\phi|k,\ell,m\rangle = R_{k\ell}(r)\,Y_{\ell m}(\theta,\phi)$$

$R_{k\ell}(r)$ e $Y_{\ell m}(\theta,\phi)$ ESTÃO NORMALIZADOS "SEPARADAMENTE":

$$\int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \; Y^*_{\ell' m'}(\theta,\phi)\,Y_{\ell m}(\theta,\phi) = \delta_{\ell\ell'}\,\delta_{mm'}$$

E:

$$\int_0^{\infty} r^2 dr \; R^*_{k'\ell}(r)\,R_{k\ell}(r) = \delta_{kk'}$$

(NOTE QUE OS ℓ'S SÃO OS MESMOS)

$$|\psi\rangle = \sum_{k=1}^{g(\ell)} \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} c_{k\ell m} |k\ell m\rangle \qquad \sum_{k\ell m} |c_{k\ell m}|^2 = 1$$

EM COORDENADAS:

$$\psi(r,\theta,\phi) = \sum_{k\ell m} c_{k\ell m} R_{k\ell}(r) Y_{\ell m}(\theta,\phi)$$

ONDE:

$$\boxed{c_{k\ell m} = \int_0^{\infty} r^2 dr \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta \, d\theta \, R^*_{k\ell}(r) Y^*_{\ell m}(\theta,\phi) \psi(r,\theta,\phi)}$$

Probabilidades de medidas de L^2 e L_z

Método 1: Supondo que temos uma base padrão $R_{kl}(r)$.

COMO $Y_{lm}(\theta, \phi)$ SÃO AUTO-FUNÇÕES DE L^2 E L_z, DOS POSTULADOS, AS PROBABILIDADES DE RESULTADOS DE MEDIDAS DE L^2 E L_z SÃO:

$$P_{L^2, L_z}(l, m) = \sum_{k=1}^{g(l)} |c_{klm}|^2$$

SUPONHAMOS MEDIDAS APENAS DE L^2:

$$P_{L^2}(l) = \sum_{k=1}^{g(l)} \sum_{m=-l}^{l} |c_{klm}|^2$$

FINALMENTE, SE EU MEDIR APENAS L_z:

$$P_{L_z}(m) = \sum_{l \geq |m|}^{\infty} \sum_{k=1}^{g(l)} |c_{klm}|^2$$

Método 2: Sem a suposição de que temos uma base $R_{kl}(r)$, podemos expandir apenas a parte angular, já que o momento angular só age nos ângulos.

DADA $\psi(r,\theta,\phi)$ PODEMOS EXPANDIR A PARTE ANGULAR:

$$\psi(r,\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_{lm}(r)\, Y_{lm}(\theta,\phi)$$

ONDE: $$a_{lm}(r) = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\; Y_{lm}^{*}(\theta,\phi)\, \psi(r,\theta,\phi)$$

COMPARANDO COM: $$\psi(r,\theta,\phi) = \sum_{klm} c_{klm}\, R_{kl}(r)\, Y_{lm}(\theta,\phi)$$

VEMOS QUE:

$$a_{lm}(r) = \sum_{k=1}^{g(l)} c_{klm} R_{kl}(r)$$ E

$$c_{klm} = \int_0^{\infty} r^2 dr\, R_{kl}^{*}(r)\, a_{lm}(r)$$ JÁ QUE:

$$c_{klm} = \int_0^{\infty} r^2 dr \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\; R_{kl}^{*}(r)\, Y_{lm}^{*}(\theta,\phi)\, \psi(r,\theta,\phi)$$

MAS, NOTE QUE:

$$\int_0^\infty r^2 dr\, |a_{lm}(r)|^2 = \int_0^\infty r^2 dr \underbrace{\sum_{k'=1}^{g(l)} C^*_{k'lm} R^*_{k'l}(r)}_{a^*_{lm}(r)} \underbrace{\sum_{k=1}^{g(l)} C_{klm} R_{kl}(r)}_{a_{lm}(r)}$$

$$= \sum_{k,k'} C^*_{k'lm} C_{klm} \underbrace{\int_0^\infty r^2 dr\, R^*_{k'l}(r) R_{kl}(r)}_{\delta_{kk'} \text{ (BASE PADRÃO)}}$$

$$= \sum_{kk'} \delta_{kk'} C^*_{k'lm} C_{klm} = \sum_{k=1}^{g(l)} |C_{klm}|^2 = P_{L^2, L_z}(l,m)$$

ASSIM! $$P_{L^2, L_z}(l,m) = \int_0^\infty r^2 dr\, |a_{lm}(r)|^2$$

ONDE: $$a_{lm}(r) = \int_0^{2\pi} d\phi \int_0^\pi \sin\theta\, d\theta\, Y^*_{lm}(\theta,\phi)\, \psi(r,\theta,\phi)$$

SE MEDIRMOS APENAS L^2:

$$P_{L^2}(\ell) = \sum_{m=-\ell}^{\ell} P_{L^2,L_z}(\ell,m) = \sum_{m=-\ell}^{\ell} \int_0^\infty r^2 dr \, |a_{\ell m}(r)|^2$$

FINALMENTE, SE EU MEDIR APENAS L_z:

$$P_{L_z}(m) = \sum_{\ell \geq |m|}^{\infty} P_{L^2,L_z}(\ell,m) = \sum_{\ell \geq |m|}^{\infty} \int_0^\infty r^2 dr \, |a_{\ell m}(r)|^2$$

Exemplos

A) $\psi(r,\theta,\phi) = f(r)\, g(\theta,\phi) \longrightarrow$ NORMALIZADA

E ASSUMIMOS QUE AS FUNÇÕES ESTÃO SEPARADAMENTE NORMALIZADAS:

$$\int_0^\infty r^2 dr\, |f(r)|\, dr = 1 = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\, |g(\theta,\phi)|^2$$

ISSO É SEMPRE POSSÍVEL [$f(r) \to N f(r)$; $g(\theta,\phi) \to \frac{1}{N} g(\theta,\phi)$]

E ESCOLHA N TAL QUE $N f(r)$ SEJA NORMALIZADA

USANDO MÉTODO <u>2</u>:

$$g(\theta,\phi) = \sum_{l,m} d_{l,m} Y_{lm}(\theta,\phi)$$ ONDE

$$d_{l,m} = \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta\, Y^*_{lm}(\theta,\phi)\, g(\theta,\phi)$$

SEGUE QUE:

$$\psi(r,\theta,\phi) = f(r)\, g(\theta,\phi) = \sum_{l,m} d_{lm}\, f(r)\, Y_{lm}(\theta,\phi)$$

COMPARANDO COM:

$$\psi(r,\theta,\phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_{lm}(r)\, Y_{lm}(\theta,\phi)$$

$$\Rightarrow a_{l,m}(r) = f(r)\, d_{l,m}$$

PORTANTO: $P_{L^2,L_z}(l,m) = \int_0^{\infty} r^2 dr\, |a_{lm}(r)|^2$

$$= \int_0^{\infty} r^2 dr\, |d_{l,m}|^2 |f(r)|^2 = |d_{l,m}|^2$$

AS OUTRAS PROBABILIDADES SEGUEM DESSA

5. A system whose state space is $\mathcal{E}_{\mathbf{r}}$ has for its wave function:

$$\psi(x, y, z) = N(x + y + z)\mathrm{e}^{-\mathbf{r}^2/\alpha^2}$$

$-e^{i\phi} + e^{-i\phi} = -2i \sin\phi$

where α, which is real, is given and N is a normalization constant.

a. The observables L_z and $\mathbf{L}^2$ are measured; what are the probabilities of finding 0 $= m$ and $2\hbar^2$? Recall that:

$\to \ell = 1$ $\qquad P_{L^2, L_z}(\ell = 1, m = 0)$

$$Y_1^0(\theta, \varphi) = \sqrt{\frac{3}{4\pi}} \cos\theta \longrightarrow \cos\theta = \sqrt{\frac{4\pi}{3}}\, Y_{1,0}(\theta, \phi)$$

b. If one also uses the fact that:

$$Y_1^{\pm 1}(\theta, \varphi) = \mp\sqrt{\frac{3}{8\pi}} \sin\theta\, \mathrm{e}^{\pm i\varphi}$$

$\sin\theta\cos\phi = \sqrt{\frac{8\pi}{3}}\left[-Y_{1,1} + Y_{1,-1}\right]\frac{1}{2}$

$\sin\theta\sin\phi = \sqrt{\frac{8\pi}{3}}\left[Y_{1,1} + Y_{1,-1}\right]\frac{1}{(-2i)}$

is it possible to predict directly the probabilities of all possible results of measurements of $\mathbf{L}^2$ and L_z in the system of wave function $\psi(x, y, z)$?

COORDENADAS ESFÉRICAS!

$$\psi(r, \theta, \phi) = \underbrace{N r e^{-r^2/\alpha}}_{f(r)} \underbrace{\left[\sin\theta\cos\phi + \sin\theta\sin\phi + \cos\theta\right]}_{g(\theta, \phi)}$$

$$\Rightarrow g(\theta,\phi) = \sin\theta\cos\phi + \sin\theta\sin\phi + \cos\theta$$

$$= \sqrt{\frac{4\pi}{3}}\, Y_{1,0} + \sqrt{\frac{2\pi}{3}}\left[-Y_{1,1} + Y_{1,-1}\right] + \sqrt{\frac{2\pi}{3}}\,(i)\left[Y_{1,1} + Y_{1,-1}\right]$$

$$= \sqrt{\frac{2\pi}{3}}\left[\sqrt{2}\, Y_{1,0} + (-1+i)\, Y_{1,1} + (1+i)\, Y_{1,-1}\right]$$

$$= \sqrt{\frac{4\pi}{3}}\left[Y_{1,0} + \frac{(-1+i)}{\sqrt{2}}\, Y_{1,1} + \frac{(1+i)}{\sqrt{2}}\, Y_{1,-1}\right] \times \frac{\sqrt{3}}{\sqrt{3}}$$

$$= \sqrt{4\pi}\,\underbrace{\left[\frac{1}{\sqrt{3}}\, Y_{1,0} + \frac{1}{\sqrt{3}}\frac{(-1+i)}{\sqrt{2}}\, Y_{1,1} + \frac{1}{\sqrt{3}}\frac{(1+i)}{\sqrt{2}}\, Y_{1,-1}\right]}_{\sum_{m=-1}^{+1} b_m Y_{1,m} = g(\theta,\phi)}$$

$$\underbrace{\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta}_{\int d\Omega}\, |g(\theta,\phi)|^2 = \int d\Omega \sum_{m'} b_{m'}^{*} Y_{1m'}^{*} \sum_{m} b_m Y_{1m}$$

$$= \sum_{m,m'} b_{m'}^{*} b_m \underbrace{\int d\Omega\, Y_{1m'}^{*} Y_{1m}}_{\delta_{m,m'}} = \sum_{m=-1}^{+1} |b_m|^2 = 1$$

$$g(\theta,\phi) = \sqrt{4\pi}\; g(\theta,\phi)$$

$$\psi(r,\theta,\phi) = \underbrace{N\sqrt{4\pi}\, r\, e^{-r^2/\alpha}}_{\substack{\text{NORMALIZADO} \\ \text{A } 1 \to f'(r)}}\; \underbrace{g(\theta,\phi)}_{\to \text{ NORMALIZADO A } 1}$$

DO MÉTODO 2:

$$\psi(r,\theta,\phi) = \sum_{l,m} f(r)\, \underbrace{d_{l,m} Y_{lm}(\theta,\phi)}_{g(\theta,\phi)} \Rightarrow \begin{cases} d_{1,0} = \frac{1}{\sqrt{3}} \\ d_{1,1} = \frac{1}{\sqrt{3}} \frac{(-1+i)}{\sqrt{2}} \\ d_{1,-1} = \frac{1}{\sqrt{3}} \frac{(1+i)}{\sqrt{2}} \end{cases}$$

$$P_{L^2,L_z}(l,m) = |d_{l,m}|^2$$

a. $P_{L^2,L_z}(l=1, m=0) = |d_{1,0}|^2 = \frac{1}{3}$

b. $P_{L^2,L_z}(l,m) = \begin{cases} l=1, m=0: 1/3 \\ l=1, m=1: 1/3 \\ l=1, m=-1: 1/3 \end{cases}$

QUALQUER OUTRO PAR (l,m):

$P_{L^2,L_z}(l,m) = 0$

SUPONHA:

$$\psi(r,\theta,\phi) = N\, e^{-r^2/a}\left[x^2+y^2-z^2\right]$$

$$P_{L^2}(\ell) = \begin{cases} \ell = 0 \rightarrow P \\ \ell = 2 \rightarrow P \end{cases}$$

$$\ell = 1, 3, 5 \ldots \rightarrow P = 0$$

SE QUISER APENAS $m=0$

$$\int d\Omega \; \underbrace{Y^*_{1,0}(\theta,\phi)}_{\cos\theta} \, \psi(r,\theta,\phi)$$

$$\int d\Omega \; Y^*_{11} \, \psi(r,\theta,\phi)$$